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Cotangent bundle reduction and Poincaré–Birkhoff normal forms

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HIGHLIGHTS

- The construction of canonical coordinates for symmetry reduced Hamiltonian systems.
- A detailed discussion of simple mechanical systems with symmetries.
- An algorithm to compute the Poincaré–Birkhoff normal form of relative equilibria.
- Example 1: a $SO(3)$ symmetry reduced three-body system.
- Example 2: a $SO(2)$ symmetry reduced double spherical pendulum.

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ABSTRACT

In this paper we study a systematic and natural construction of canonical coordinates for the reduced space of a cotangent bundle with a free Lie group action. The canonical coordinates enable us to compute Poincaré–Birkhoff normal forms of relative equilibria using standard algorithms. The case of simple mechanical systems with symmetries is studied in detail. As examples we compute Poincaré–Birkhoff normal forms for a Lagrangian equilateral triangle configuration of a three-body system with a Morse-type potential and the stretched-out configuration of a double spherical pendulum.

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1. Introduction

The theory of the reduction of Hamiltonian systems with symmetry is well developed [1,2]. Although it is a classical subject and goes back to the pioneers of mechanics, a modern theory was only established in the 1970s. The main idea can be summarized as follows.

Let P be a symplectic manifold with a symmetry group G , and let $J : P \rightarrow \mathfrak{g}^*$ be an equivariant *momentum mapping* with respect to the coadjoint action of G on \mathfrak{g}^* , where \mathfrak{g}^* is the dual space of the Lie algebra \mathfrak{g} of G . Then, under some regularity conditions, the reduced space given by the quotient space $P_\mu := J^{-1}(\mu)/G_\mu$, where G_μ is the isotropy group of $\mu \in \mathfrak{g}^*$, is a symplectic manifold. A G -invariant Hamiltonian function on P can be reduced to a function on P_μ which generates the reduced dynamics.

The algebraic definition as a quotient makes it often difficult to explicitly construct the reduced space P_μ and develop a good

intuition for it. For example, P_μ is not necessarily a linear space even if P is linear. This is the case, for example, in the n -body problem: Although the translation reduced space is Euclidean, the reduced space of rotations is in general not linear [3]. But as the reduced space is a symplectic manifold it follows from the Darboux theorem that one can locally construct canonical coordinates so that the reduced space locally becomes a linear symplectic space. Such canonical coordinates are very useful. For example, they form the starting point of standard algorithms for the computation of the Poincaré–Birkhoff normal form at an equilibrium point of a Hamiltonian system [4–8]. A Poincaré–Birkhoff normal form is a main tool for the construction of center manifolds and the study of bifurcations [9]. As an example of the former application we mention the construction of the phase space structures which govern reaction dynamics induced by saddle type equilibrium points [10,11].

The main objectives of this paper are twofold. The first objective is the systematic construction of canonical coordinates for the reduced space P_μ in the case where P is a cotangent bundle and the action of G on P is free. This construction is uniform in the sense that Abelian and non-Abelian symmetries are treated on the same footing. The second objective is to illustrate how the canonical

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coordinates on the reduced space can be used to compute Poincaré–Birkhoff normal forms at relative equilibria, i.e. the equilibria of the reduced system. This has numerous applications. An example is the construction of the phase space structures which govern reactions in rotating molecules where the reaction dynamics is induced by saddle type relative equilibria [12]. To elaborate on the rich field of applications in molecular dynamics we mention as an extension of the work on point particle systems in [12] the study of systems of rigid bodies which can be used to model molecular complexes [13]. Many more examples can be given to prove the need to combine symmetry reduction with Hamiltonian normal forms. The literature on both symmetry reduction and normal forms is huge. In this paper we try to distill the most important aspects from either field that are necessary to combine the two.

We note that the computation of canonical coordinates for a reduced space of a symplectic manifold in general [14,15] or for specific cases such as, e.g., a cotangent bundle [16,17] and more concretely for n -body systems [3,18] have at least implicitly been studied in the literature before. However, for obtaining the nonlinear terms of a Poincaré–Birkhoff normal form these works have to be put into context, and a systematic study is missing. Also the work on the computations of Poincaré–Birkhoff normal forms of symmetry reduced Hamiltonians is mainly restricted to Abelian Lie group actions. In this paper we present a systematic approach which covers both the Abelian and the non-Abelian case in a uniform way.

In the following we give a brief review of the existing literature related to this paper. In order to obtain canonical coordinates on the reduced space of a cotangent bundle with a Lie group action we follow the method given in [16,17] which take a Lagrangian respectively Poisson reduction point of view. A detailed survey on cotangent bundle reduction and its history can be found in [19]. For the special case of the three-body reduction, our main references are [20,3] to which we will come back in Section 4. As for the Poincaré–Birkhoff normal form, one can find a detailed introduction in [21]. One of the first applications of the normal form theory to reduced spaces of symplectic spaces with a continuous symmetry can be found in [22] where the symmetry group is the circle group. An application to the restricted three-body problem can be found in [23,24], for instance. In [25] normal form computations are done at Lagrange points by using a splitting method. In another recent work [26] one can find a detailed study of normal form for planetary systems. Normal form at relative equilibrium of a general dynamical system are discussed in [27]. A recent review of normal form theory in dynamical systems can be found in [8].

This paper is organized as follows. We start with a general review of the action of Lie groups on tangent and cotangent bundles in Section 2. This mainly serves to introduce some basic material and settle the notation. Section 3 comprises the main result of this paper which is a systematic construction of canonical coordinates for the reduced space of a cotangent bundle with a free action of a symmetry group. This includes the derivation of the reduced Hamiltonian in canonical coordinates, a discussion of special cases like Abelian symmetry groups and systems with vanishing angular momenta in Section 3.3, a detailed discussion of the case of simple mechanical systems (Section 3.4), and the Poincaré–Birkhoff normal form of relative equilibria in Section 3.6. Section 4 contains our first example which consists of the three-body reduction. We review in this section how to derive a reduced Hamiltonian in canonical coordinates in a way which does not depend on the choice of a body-fixed reference frame, i.e. in the language of Littlejohn and Reinsch [3] in a gauge independent way. In Section 4.3 we consider a Lagrangian equilateral triangle relative equilibrium, and we compute a Poincaré–Birkhoff normal form at such configurations. In Section 5 we study our second example which is the double spherical pendulum. After obtaining canonical coordinates for the reduced system, a normal form computation is done at the relative equilibrium given by the so called stretched-out solution. Conclusions are given in Section 6.

2. Lie group actions on tangent and cotangent bundles

In this section we recall (mainly to introduce some notation) the symplectic actions of Lie groups on tangent and cotangent bundles over a configuration space. For the details, we refer to [28,1,2,29].

Let G be a Lie group and let M be a manifold which is called the *configuration space*. Let the map

$$G \times M \rightarrow M \quad (1)$$

$$(g, s) \rightarrow gs \quad (2)$$

be a free and proper action of G on M . We denote the left-translation which for a fixed $g \in G$, maps $s \in M$ to gs by L_g . The derived maps of L_g are denoted as follows. For $s \in M$, $(L_g)_* : T_s M \rightarrow T_{gs} M$ stands for the derivative map of L_g , and $(L_g)^* : T_s^* M \rightarrow T_{g^{-1}s}^* M$ stands for the pull-back map of L_g . Let \mathfrak{g} denote the Lie algebra of G . Then for $\zeta \in \mathfrak{g}$, the corresponding *infinitesimal generator* or *fundamental vector field* ζ_M at $s \in M$ is defined by

$$\zeta_M(s) = \left. \frac{d}{dt} \right|_{t=0} (L_{\exp(t\zeta)} s). \quad (3)$$

The G orbit through $s \in M$ is given by $Gs = \{gs | g \in G\} \subset M$. The fundamental vector fields ζ_M are tangent to the orbits Gs for all $s \in M$. Moreover, the tangent space $T_s(Gs)$ is spanned by the fundamental vector fields at s .

We note that if $M = G$, i.e. the action is the group operation of G , then the fundamental vector fields at $g \in G$ are given by

$$\zeta_G(g) = (R_g)_* \zeta, \quad (4)$$

where $\zeta \in \mathfrak{g}$ and R_g is the right-translation by g [1].

The coadjoint action of G on the dual space \mathfrak{g}^* of its Lie algebra is defined as

$$\langle (Ad_{g^{-1}})^* \mu, \zeta \rangle = \langle \mu, Ad_{g^{-1}} \zeta \rangle, \quad (5)$$

for $g \in G$, $\mu \in \mathfrak{g}^*$ and $\zeta \in \mathfrak{g}$. Here \langle, \rangle stands for the pairing between a co-vector and vector and

$$Ad_g \zeta = \left. \frac{d}{dt} \right|_{t=0} (g(\exp(t\zeta))g^{-1}) \quad (6)$$

is the adjoint action. The action on M can be lifted to TM and T^*M by the derived maps and both of the lifted actions are free when the action on M is free. The lifted action on the cotangent bundle is symplectic with respect to the natural symplectic structure on T^*M [28] and has a *momentum mapping* $J : T^*M \rightarrow \mathfrak{g}^*$ defined as

$$\langle J(s, p), \zeta \rangle = \langle p, \zeta_M(s) \rangle, \quad (7)$$

for $(s, p) \in T^*M$. It is well-known that J is equivariant with respect to the action of G on T^*M and the coadjoint action of G on \mathfrak{g}^* [28,1].

If M is a Riemannian manifold with a Riemannian metric k which is invariant under the action of G , then the lifted action on TM is also symplectic with respect to the symplectic structure induced by the one on T^*M and the corresponding momentum mapping \mathbf{L} is defined as

$$\langle \mathbf{L}(s, v), \zeta \rangle = v^T k \zeta_M(s), \quad (8)$$

for $(s, v) \in TM$ [2].

3. Canonical coordinates in cotangent bundle reduction

In this section we will obtain canonical coordinates on the symmetry reduced space. To this end we will use a coordinate-based approach to express cotangent bundle reduction in terms of the orbit reduction scheme by Marle [30,29]. A more detailed explanation of the notions used in the following subsection can be found, e.g., in [16,17,31].

3.1. Reduction of the equations of motion

The *shape space* or *internal space* Q is defined as the quotient M/G . As we assume that the action of G on M is free it follows from standard theorems that M/G has a manifold structure and $M \rightarrow Q$ is a fiber bundle [1]. Using the fiber bundle structure one can locally obtain a coordinate system on M by choosing a local coordinate system on $Q \times G$. Let us assume that a point in $Q \times G$ has coordinates (q, g) . The coordinates q are called *shape coordinates* or *internal coordinates*. Then by the decomposition [16]

$$T(Q \times G) \cong TQ \times G \times \mathfrak{g} \quad (9)$$

a point in TM has coordinates (q, \dot{q}, g, \dot{g}) . Now consider the *body angular velocity* defined by

$$\xi = (L_{g^{-1}})_* \dot{g}, \quad (10)$$

where $(L_{g^{-1}})_*$ denotes the differential of the left translation $L_{g^{-1}} : G \rightarrow G, h \mapsto g^{-1}h$, at the unit element of G . The commonly used notion of body angular velocity comes from the fact that in the example where G is the rotational symmetry group $SO(3)$ (see Section 4) ξ is indeed the angular velocity in a body fixed frame. We note that Eq. (10) is called the *reconstruction equation* as it can be used to find the full dynamics corresponding to the reduced one [2].

The key point in reduction is to note that the body angular velocity is invariant under the group action. Namely, for $h \in G$, define the curve $m(t) = hg(t)$. Then

$$(L_{m^{-1}})_* \dot{m} = (L_{(g^{-1}h^{-1})})_* ((L_h)_* \dot{g}) = \xi. \quad (11)$$

As ξ is invariant under the group action, the coordinates (q, \dot{q}, ξ) give a coordinate system on $(TM)/G$.

Let $L : TM \rightarrow \mathbb{R}$ be a *regular* Lagrangian function, i.e. a function for which the Legendre transform $\mathbb{F}L : TM \rightarrow T^*M$ defined as

$$\mathbb{F}L(m, v) = \frac{\partial L}{\partial v}(m, v) \quad (12)$$

is regular for all $m \in M$ and $v \in T_m M$ [1]. Further assume that L is invariant under the action of G . Then the function $l : TM/G \rightarrow \mathbb{R}$ given by

$$l(q, \dot{q}, \xi) := L(q, \dot{q}, g, \dot{g}) \quad (13)$$

is well-defined. This is done by passing to the coordinates (q, \dot{q}, ξ) , and as the Lagrangian L is invariant, it is possible to put L in the form of the function l in which the G coordinates disappear. Using l we can define momenta conjugate to q and ξ as

$$p_q = \frac{\partial l}{\partial \dot{q}}, \quad (14)$$

and

$$\eta = \frac{\partial l}{\partial \xi}, \quad (15)$$

respectively. Here η is called the *body angular momentum*, and by the chain rule,

$$\eta = (L_g)_* p_g, \quad (16)$$

where $p_g = \partial L / \partial \dot{g}$ is the conjugate momentum of $g \in G$ [32]. Like body angular velocity the notion body angular momentum again comes from the context of reduction of rotational symmetries. Similarly to the decomposition (9) we locally have

$$T^*M \cong T^*Q \times G \times \mathfrak{g}^* \quad (17)$$

with coordinates (q, p_q, g, p_g) . Similarly to the body angular velocity the body angular momentum is invariant under the group action. Hence we can view (q, p_q, η) as coordinates on T^*M/G .

Let $H : T^*M \rightarrow \mathbb{R}$ be the Hamiltonian obtained from the Legendre transformation $\mathbb{F}L$ of the Lagrangian L [1], i.e., in coordinates

$$H(q, p_q, g, p_g) = \dot{q}p_q + \dot{g}p_g - L(q, \dot{q}, g, \dot{g}). \quad (18)$$

If L is invariant with respect to the action of G on TM then H is invariant with respect to the action of G on T^*M and induces a function h on T^*M/G given by

$$h(q, p_q, \eta) := H(q, p_q, g, p_g). \quad (19)$$

From the construction above one obtains for the momentum mapping J in (7) at $z = (q, p_q, g, p_g)$ and for $\zeta \in \mathfrak{g}$,

$$\begin{aligned} \langle J(z), \zeta \rangle &= \langle (p_q, p_g), \zeta_M \rangle \\ &= \langle (p_q, p_g), (0, (R_g)_* \zeta) \rangle \\ &= \langle p_g, (R_g)_* \zeta \rangle \\ &= \langle (L_{g^{-1}})^* \eta, (R_g)_* \zeta \rangle \\ &= \langle (Ad_{g^{-1}})^* \eta, \zeta \rangle. \end{aligned} \quad (20)$$

Here the first equality follows from the definition of the momentum map (7), the second equality makes use of the decomposition (9), the fact that ζ_M is tangent to the group orbit which we identify with G and (4), the third equality is clear, the fourth equality uses (16) and the final equality follows from the definition of the coadjoint action in (5) and (6).

We thus obtain

$$J(z) = (Ad_{g^{-1}})^* \eta \quad (21)$$

or equivalently

$$\eta = (Ad_g)^* J(z). \quad (22)$$

Let \mathcal{O}_μ stand for the coadjoint orbit through $J(z) = \mu \in \mathfrak{g}^*$ for some fixed $\mu \in \mathfrak{g}^*$, i.e.

$$\mathcal{O}_\mu = \{(Ad_{g^{-1}})^* \mu | g \in G\} \subset \mathfrak{g}^*. \quad (23)$$

Then Eq. (22) gives that

$$\eta \in \mathcal{O}_\mu. \quad (24)$$

As J is equivariant, it induces a map $j : T^*M/G \rightarrow \mathfrak{g}^*/G$. Now consider the *reduced space*

$$P_\mu := j^{-1}(\mathcal{O}_\mu). \quad (25)$$

By (24), we conclude that if $J(z) = \mu$ for $z = (q, p_q, g, p_g)$ and some fixed $\mu \in \mathfrak{g}^*$, then for $\eta = (Ad_g)^* J(z)$, we have $(q, p_q, \eta) \in P_\mu$, i.e. (q, p_q, η) are coordinates on the reduced space.

The reduction to the space P_μ we described is a coordinate-based form of the *orbit reduction* of Marle [29]. For n -body systems, the reduction procedure can be interpreted as passing to a *body-fixed frame* (cf. Section 4). In fact, the space P_μ is symplectomorphic to the *Marsden–Weinstein reduced space* $J^{-1}(\mu)/G_\mu$, where G_μ is the isotropy group of $\mu \in \mathfrak{g}^*$. For us, the reduced space P_μ and the coordinates (q, p_q, η) form the basis for defining canonical coordinates on the reduced phase space.

3.2. Canonical coordinates

The coordinates (q, p_q, g, p_g) defined above are clearly canonical, whereas the coordinates (q, p_q, g, η) (as we will see below) are not canonical. By (14) and (15) we get the Poisson bracket equalities

$$\{q_\alpha, \eta_a\} = \{p_{q_\alpha}, \eta_a\} = 0 \quad (26)$$

on T^*M for all α and a . Now recall the identification $\xi = (L_{g^{-1}})_* \dot{g}$, and let (e_1, \dots, e_l) be a basis of \mathfrak{g} , where l is the dimension of G .

Choosing $(q_\alpha, \dot{q}_\alpha, g_a, \dot{g}_a)$ in place of $(q_\alpha, \dot{q}_\alpha, g_a, \dot{g}_a)$ as coordinates on TM we get that [3]

$$\{\eta_a, \eta_b\} = -\gamma_{ab}^c \eta_c, \quad (27)$$

where γ_{ab}^c are the structure constants given by $[e_a, e_b] = \gamma_{ab}^c e_c$. This is in fact the same as the $(-)$ Lie–Poisson bracket [2] on G . As the Poisson structure on the coadjoint orbit \mathcal{O}_μ is the reduced one from the Lie–Poisson structure on G , the discussion above suggests that if a canonical coordinate system (u, v) is chosen on \mathcal{O}_μ such that

$$\eta = \eta(u, v), \quad (28)$$

then the coordinate system (q, p_q, u, v) becomes a canonical coordinate system on P_μ .

For a more detailed discussion of canonical coordinates on coadjoint orbits, we refer to [33] among others. In our example of the three body-problem in Section 4 the coadjoint orbits are the body-angular momentum spheres. In this case the canonical coordinates may be chosen as *Deprit coordinates* [34] on the body-angular momentum sphere (see (87) below).

As for the dynamics, if one passes to the coordinates given in (28), then the reduced Hamiltonian $h_\mu := h|_{P_\mu}$ may be written in the form

$$h_\mu = h_\mu(q, p_q, u, v). \quad (29)$$

Then the equations of motion for the reduced system have the familiar form

$$\dot{z} = \{z, h_\mu\} \quad (30)$$

for $z = (q, p_q, u, v)$.

Remark 3.1. It is known that the reduced space $P_\mu = J^{-1}(\mathcal{O}_\mu)/G$ is locally diffeomorphic to $T^*(M/G) \times \mathcal{O}_\mu$ but the symplectic structure on the reduced space is not the sum of the canonical symplectic structures on $T^*(M/G)$ and \mathcal{O}_μ [29]. Without going into details we note that the canonical structure is indeed much more involved [29]. However by passing to canonical coordinates the Poisson structure on the reduced space has standard form.

3.3. Special cases

(1) *G is Abelian.* Consider the case where the Lie group is Abelian, e.g. a torus group. The reduction strongly simplifies in this case. Since the coadjoint action is trivial the well-known identification [29]

$$J^{-1}(\mathcal{O}_\mu)/G = T^*Q \quad (31)$$

is obtained. This shows that one can take the coordinates (q^α, p_q^α) as the canonical coordinates on the reduced space, which is symplectomorphic to T^*Q . An example of this situation is given by the translational motions of an n -body system [3]. We will explicitly illustrate the Abelian case for the example of a double spherical pendulum in Section 5. A detailed analysis of the Abelian case in the Lagrangian setting can be found in [16].

(2) *Vanishing angular momentum.* With the notation above, if $\eta \equiv 0$, then the coadjoint orbit is trivial as in the first special case. Then the reduced space is symplectomorphic to T^*Q . A well studied example of a system with vanishing angular momentum is the so called *falling cat problem* [35].

(3) *Generalized rigid bodies.* Suppose that $M = G$. Then Q is just a point and

$$J^{-1}(\mathcal{O}_\mu)/G = \mathcal{O}_\mu. \quad (32)$$

This occurs, e.g., for a rigid body, where the configuration space M is the rotation group $SO(3)$ and the reduced space is the body-angular momentum sphere.

3.4. Simple mechanical systems

The construction of canonical coordinates on the reduced phase space and the reduction of the equations of motion can be described more explicitly in the case of simple mechanical systems. For a simple mechanical system with a Lie symmetry group G , the Lagrangian is of the form

$$L(s, \dot{s}) = \frac{1}{2} \dot{s}^T k \dot{s} - V(q), \quad (33)$$

where s is a coordinate system on M , k is a Riemannian metric on M which is invariant under the action of G on M , and V is a potential function which is also invariant and hence, if (q, g) is a coordinate system on the local trivialization

$$M \cong Q \times G \quad (34)$$

then V depends only on the shape coordinates q . The term $\frac{1}{2} \dot{s}^T k \dot{s}$ is the kinetic energy which we will denote by K .

Let $\sigma : Q \rightarrow M$ be a local section of the fiber bundle, i.e. σ is a right inverse of the projection $\pi : M \rightarrow Q$. If a point $q \in Q$ is given, then a point $s \in \pi^{-1}(q)$ is of the form $g\sigma(q)$ with some $g \in G$. Set $r = \sigma(q)$, then

$$\dot{s} = \frac{\partial r}{\partial q} \dot{q} \quad (35)$$

by the chain rule.

Let the *body velocities* be defined as

$$v = (L_{g^{-1}})_* \dot{s}. \quad (36)$$

By using the Leibniz rule [1] and the definition of the fundamental vector field one obtains

$$v = \xi_M(r) + \dot{r}, \quad (37)$$

where ξ_M is the fundamental vector field corresponding to $\xi = (L_{g^{-1}})_* \dot{g} \in \mathfrak{g}$. The kinetic energy thus becomes

$$K = \frac{1}{2} v^T k v = \frac{1}{2} \xi_M(r)^T k \xi_M(r) + \xi_M(r)^T k \dot{r} + \frac{1}{2} \dot{r}^T k \dot{r}. \quad (38)$$

For $\xi, \zeta \in \mathfrak{g}$, set

$$\xi^T \mathbb{I} \zeta = \xi_M(r)^T k \zeta_M(r). \quad (39)$$

Then \mathbb{I} is a left-invariant inner product on \mathfrak{g} [2]. For $G = SO(3)$ (respectively $\mathfrak{g} = \mathfrak{so}(3)$), \mathbb{I} is the moment of inertia tensor (see Section 4). In order to decouple the kinetic energy in group and shape terms, the so called *mechanical connection* is introduced [2]. The mechanical connection $A : TM \rightarrow \mathfrak{g}$ is defined as

$$A(s, \dot{s}) = \mathbb{I}^{-1} \mathbf{L}(s, \dot{s}), \quad (40)$$

where \mathbf{L} is the momentum map given in (8), and $\mathbb{I}^{-1} : \mathfrak{g}^* \rightarrow \mathfrak{g}$ is the linear map associated with the inner product \mathbb{I} . At any point $s \in M$, the tangent space to $T_s M$ may be decomposed as

$$T_s M = V_s + H_s, \quad (41)$$

where V_s is the tangent space to the orbit Gs , and H_s is the space which is orthogonal to V_s with respect to the metric k . A tangent vector $w \in T_s M$ may be written in this decomposition as

$$w = \text{ver}_s w + \text{hor}_s w. \quad (42)$$

It turns out that [2]

$$\text{ver}_s w = [A(s, w)]_M(s) \quad (43)$$

and

$$\mathbf{L}(s, \text{hor}_s w) = 0. \quad (44)$$

With respect to this decomposition \dot{r} may be written in the form

$$\dot{r} = \text{ver } \dot{r} + (\dot{r} - \text{ver } \dot{r}). \quad (45)$$

If a new metric d is introduced by

$$\dot{q}^T d \dot{q} := (\dot{r} - \text{ver } \dot{r})^T k (\dot{r} - \text{ver } \dot{r}), \quad (46)$$

which is called the *horizontal metric*, and if we define the map $A_Q : TQ \rightarrow \mathfrak{g}$ by

$$A_Q \dot{q} := A \dot{r}, \quad (47)$$

then after rearranging terms the kinetic energy assumes the form

$$K = \frac{1}{2} (\xi + A_Q \dot{q})^T \mathbb{I} (\xi + A_Q \dot{q}) + \frac{1}{2} \dot{q}^T d \dot{q}. \quad (48)$$

This compact form of the kinetic energy reflects the decomposition of it into vertical and horizontal energies. Finally the Lagrangian in coordinates (q, \dot{q}, ξ) is given by

$$l(q, \dot{q}, \xi) = \frac{1}{2} (\xi + A_Q \dot{q})^T \mathbb{I} (\xi + A_Q \dot{q}) + \frac{1}{2} \dot{q}^T d \dot{q} - V(q). \quad (49)$$

If the *body angular momentum* is defined by

$$\mathbf{J} = (L_{g^{-1}})_* \mathbf{L}, \quad (50)$$

then it is seen that

$$\mathbf{J} = \mathbb{I} (\xi + A_Q \dot{q}). \quad (51)$$

On the other hand, the conjugate momenta of q and ξ are obtained as

$$p_q = \frac{\partial l}{\partial \dot{q}} = d \dot{q} + A_Q^T \mathbf{J}, \quad (52)$$

and

$$\eta = \frac{\partial l}{\partial \xi} = \mathbb{I} (\xi + A_Q \dot{q}), \quad (53)$$

respectively. Note here that $\eta = \mathbf{J}$. Finally the Hamiltonian can be written as

$$h(q, p_q, \mathbf{J}) = \frac{1}{2} \mathbf{J}^T \mathbb{I}^{-1} \mathbf{J} + (p_q - A_Q^T \mathbf{J})^T d^{-1} (p_q - A_Q^T \mathbf{J}) + V(q), \quad (54)$$

where d^{-1} denotes the metric on T^*M corresponding to d . This Hamiltonian is an extension of the N -body ro-vibrational Hamiltonian in [3] to general simple mechanical systems.

Remark 3.2. Eq. (52) shows that due to the presence of magnetic-like terms the momenta p_q corresponding to the shape space coordinates q do not belong to the cotangent space $T^*(M/G)$ [29]. This point clarifies what is noted in Remark 3.1.

3.5. Relative equilibria of simple mechanical systems

A point in T^*M is called a *relative equilibrium point* if its projection into the reduced space is a critical point of the reduced Hamiltonian. So we are interested in the equilibria of the function $h_\mu : P_\mu \rightarrow \mathbb{R}$ for some fixed $\mu \in \mathfrak{g}^*$. We will give some criteria for relative equilibria for simple mechanical systems.

From Eq. (54) the equations of motion are obtained to be [3,36,37,15,38]

$$\begin{aligned} \dot{\mathbf{J}} &= -\text{ad}_{\partial h / \partial \mathbf{J}}^* \mathbf{J} \\ \dot{q} &= \frac{\partial h}{\partial p_q} = d^{-1} (p_q - A_Q^T \mathbf{J}), \\ \dot{p}_q &= -\frac{\partial h}{\partial q} = -\frac{1}{2} \frac{\partial}{\partial q} ((p_q - A_Q^T \mathbf{J})^T d^{-1} (p_q - A_Q^T \mathbf{J})) + \frac{\partial V_{\text{eff}}}{\partial q}, \end{aligned} \quad (55)$$

where

$$\frac{\partial h}{\partial \mathbf{J}} = \mathbb{I}^{-1} \mathbf{J} - A_Q d^{-1} (p_q - A_Q^T \mathbf{J}) \quad (56)$$

and

$$V_{\text{eff}} = \frac{1}{2} \mathbf{J}^T \mathbb{I}^{-1} \mathbf{J} + V(q) \quad (57)$$

is the *effective potential* which, for Abelian actions, agrees with the so called *amended potential* [2,39,40].

Then the conditions for having a relative equilibrium are

$$\begin{aligned} p_q &= A_Q^T \mathbf{J}, \\ \text{ad}_{\mathbb{I}^{-1} \mathbf{J}}^* \mathbf{J} &= 0, \\ \frac{\partial}{\partial q} V_{\text{eff}} &= 0. \end{aligned} \quad (58)$$

In the examples of the three-body problem and the double spherical pendulum in Sections 4 and 5 the conditions will be given in a more explicit form.

3.6. Poincaré–Birkhoff normal form at a relative equilibrium point

The Poincaré–Birkhoff normal form is a main tool in dynamical systems theory. It allows one (if certain conditions are satisfied) to study the dynamics of a nonlinear system in the neighborhood of an equilibrium point by approximating it by a ‘simpler’ system. This has many applications, e.g., in the study of bifurcations and the computations of center manifolds [4–7]. The simpler system is constructed order by order of the Taylor expansion of the original system at the equilibrium point by a suitable choice of coordinates at each order. For Hamiltonian systems, the coordinate transformations are sought to be symplectic. As the dynamics (i.e. the vector field) is generated by a Hamilton function the simplification can be described completely in terms of a simplification of the Hamilton function. There are well established algorithms which can be implemented on a computer and which allow one to compute normal forms to any desired order. As the starting point for these algorithms is a Hamiltonian system with canonical coordinates on the linear symplectic space $\mathbb{R}^f \times \mathbb{R}^f$ where f denotes the number of degrees of freedom it is crucial for the application of these algorithms to relative equilibria of symmetry reduced Hamiltonian systems to explicitly construct canonical coordinates on the reduced space as described in the subsections above.

We will in this paper restrict ourselves to Poincaré–Birkhoff normal forms at equilibrium points where the eigenvalues associated with the linearized Hamiltonian vector field $\mathfrak{J} D^2 H$ are purely imaginary. Here \mathfrak{J} denotes the standard symplectic matrix and $D^2 H$ is the Hessian of the Hamiltonian H . We will denote the eigenvalues by $\pm i \omega_k$, $k = 1, \dots, f$. Assuming that the eigenvalues are independent over the field of rational numbers (i.e. in the absence of *resonances*), the Poincaré–Birkhoff normal form yields a symplectic transformation to new (*normal form*) coordinates such that the transformed Hamiltonian function truncated at order n_0 of its Taylor expansion assumes the form

$$H_{\text{NF}}(I_1, \dots, I_f) = \sum_{k=1}^f \omega_k I_k + \text{h.o.t.}, \quad (59)$$

where I_k , $k = 1, \dots, f$, are constants of motions which (when expressed in terms of the normal form coordinates) have the form

$$I_k = p_k^2 + q_k^2, \quad k = 1, \dots, f, \quad (60)$$

and H_{NF} is a polynomial of order $n_0/2$ in I_k , $k = 1, \dots, f$ and hence of order n_0 in p and q (note that only even orders n_0 of a normal form make sense). The algorithm to compute this transformation is given in [41]. We will apply it to the examples of relative

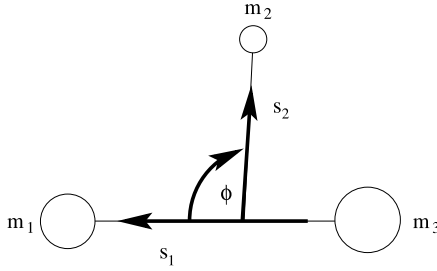


Fig. 1. Definition of the Jacobi vectors \mathbf{s}_1 and \mathbf{s}_2 and the corresponding angle ϕ .

equilibria of a three-body system and a double spherical pendulum in Sections 4.3 and 5.3, respectively.

4. Three-body systems

In this section we review the reduction of a three-body system for which we then write the reduced Hamiltonian in canonical coordinates following Section 3 (see also [12]). As an example we discuss a triatomic molecule with a Morse-type potential for which we compute the Poincaré–Birkhoff normal form about an equilibrium point given by an equilateral triangle configuration.

4.1. Reduced equations of motion

Consider a system of three bodies with masses m_1, m_2, m_3 and position vectors $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3 \in \mathbb{R}^3$, respectively, without external forces acting on the three bodies. The symmetry of overall translations can be reduced by introducing mass-weighted Jacobi vectors which are defined as

$$\begin{aligned}\mathbf{s}_1 &= \sqrt{\mu_1}(\mathbf{x}_1 - \mathbf{x}_3), \\ \mathbf{s}_2 &= \sqrt{\mu_2} \left(\mathbf{x}_2 - \frac{m_1\mathbf{x}_1 + m_3\mathbf{x}_3}{m_1 + m_3} \right),\end{aligned}$$

where

$$\mu_1 = \frac{m_1 m_3}{m_1 + m_3}, \quad \mu_2 = \frac{m_2(m_1 + m_3)}{m_1 + m_2 + m_3} \quad (61)$$

are reduced masses (see Fig. 1).

Excluding collinear (and hence also collisional) configurations we obtain the six-dimensional translation-reduced configuration space

$$M = \{s = (\mathbf{s}_1, \mathbf{s}_2) : \lambda \mathbf{s}_1 + \mu \mathbf{s}_2 \neq 0 \text{ for all } (\lambda, \mu) \in \mathbb{R}^2 \setminus \{0\}\} \subset \mathbb{R}^3 \times \mathbb{R}^3. \quad (62)$$

Proper rotations $g \in SO(3)$ act on M in the natural way

$$g(\mathbf{s}_1, \mathbf{s}_2) = (g\mathbf{s}_1, g\mathbf{s}_2). \quad (63)$$

On M this action is free and it thus follows that the shape space

$$Q := M/SO(3) \quad (64)$$

has a manifold structure which turns out to be diffeomorphic to $\mathbb{R}_+^3 = \{(x, y, z) \in \mathbb{R}^3 : z > 0\}$ [20]. The canonical projection $M \rightarrow Q$ defines a principal bundle with structure group $SO(3)$. This principal bundle is trivial [20] and has holonomy group $SO(2)$ yielding a geometric reduction [42].

The Lie algebra $\mathfrak{g} = \mathfrak{so}(3)$ of $G = SO(3)$ can be identified with \mathbb{R}^3 where the Lie algebra structure becomes the vector product ‘ \times ’. By using the bi-invariant inner product on \mathfrak{g} , or equivalently the dot product on \mathbb{R}^3 , one can identify \mathfrak{g}^* also with \mathbb{R}^3 . With these identifications the fundamental vector field corresponding to $\zeta \in \mathfrak{g}$ at $s = (\mathbf{s}_1, \mathbf{s}_2)$ is

$$\zeta(s) = (\zeta \times \mathbf{s}_1, \zeta \times \mathbf{s}_2). \quad (65)$$

The momentum mapping $\mathbf{L} : TM \rightarrow \mathfrak{g}^*$, following (8), is given by

$$\mathbf{L} = \mathbf{s}_1 \times \dot{\mathbf{s}}_1 + \mathbf{s}_2 \times \dot{\mathbf{s}}_2. \quad (66)$$

After choosing a body-fixed frame one can obtain the corresponding body-fixed Jacobi vectors by

$$\mathbf{s}_i = g \mathbf{r}_i, \quad i = 1, 2, \quad (67)$$

where $g \in SO(3)$ is the matrix relating the body-fixed frame and the space-fixed frame. As g depends on three coordinates, e.g. Euler angles, there are three shape space coordinates q_α , $\alpha = 1, 2, 3$, remaining to parametrize the two vectors \mathbf{r}_1 and \mathbf{r}_2 .

The kinetic energy is given by

$$K = \frac{1}{2} \sum_{i=1}^3 m_i \dot{\mathbf{x}}_i^2 = \frac{1}{2} \sum_{i=1}^2 \dot{\mathbf{s}}_i^2. \quad (68)$$

The corresponding metric k thus is Euclidean. Defining body velocities according to

$$\mathbf{v}_i = g^T \dot{\mathbf{s}}_i, \quad i = 1, 2, \quad (69)$$

(cf. (36)), and using the shape coordinates and their time derivatives one can rewrite the body velocities as

$$\begin{aligned}\mathbf{v}_i &= g^T \left(\dot{g} \mathbf{r}_i + \sum_{\alpha=1}^3 g \frac{\partial \mathbf{r}_i}{\partial q_\alpha} \dot{q}_\alpha \right) \\ &= g^T \dot{g} \mathbf{r}_i + \sum_{\alpha=1}^3 \frac{\partial \mathbf{r}_i}{\partial q_\alpha} \dot{q}_\alpha.\end{aligned}$$

The body angular velocity ξ is the vector in \mathbb{R}^3 corresponding to $\Xi \in \mathfrak{g}$ given by

$$\Xi = g^T \dot{g}, \quad (70)$$

which is the reconstruction equation (10). Then one has

$$\mathbf{v}_i = \xi \times \mathbf{r}_i + \sum_{\alpha=1}^3 \frac{\partial \mathbf{r}_i}{\partial q_\alpha} \dot{q}_\alpha \quad (71)$$

which corresponds to the general expression (37). Since the moment of inertia tensor \mathbb{I} is given by

$$\mathbb{I} \mathbf{u} = \mathbf{r}_1 \times (\mathbf{u} \times \mathbf{r}_1) + \mathbf{r}_2 \times (\mathbf{u} \times \mathbf{r}_2), \quad (72)$$

for $\mathbf{u} \in \mathbb{R}^3$, the mechanical connection $A_Q = \begin{bmatrix} \mathbf{A}_1 \\ \mathbf{A}_2 \\ \mathbf{A}_3 \end{bmatrix}$ is obtained to be

$$\mathbf{A}_\alpha = \mathbb{I}^{-1} \left(\mathbf{r}_1 \times \frac{\partial \mathbf{r}_1}{\partial q_\alpha} \right) + \mathbb{I}^{-1} \left(\mathbf{r}_2 \times \frac{\partial \mathbf{r}_2}{\partial q_\alpha} \right). \quad (73)$$

Then the kinetic energy becomes

$$K = \frac{1}{2} \xi^T \mathbb{I} \xi + \sum_{\alpha=1}^3 (\xi^T \mathbb{I} \mathbf{A}_\alpha) \dot{q}_\alpha + \frac{1}{2} \sum_{\alpha, \beta=1}^3 h_{\alpha\beta} \dot{q}_\alpha \dot{q}_\beta, \quad (74)$$

where

$$h_{\alpha\beta} = \sum_{i=1}^2 \frac{\partial \mathbf{r}_i}{\partial q_\alpha}^T \frac{\partial \mathbf{r}_i}{\partial q_\beta}. \quad (75)$$

Using that the horizontal metric is

$$d_{\alpha\beta} = h_{\alpha\beta} - \mathbf{A}_\alpha^T \mathbb{I} \mathbf{A}_\beta \quad (76)$$

(see (46)) allows one to write the kinetic energy in the compact form

$$K = \frac{1}{2} \sum_{\alpha, \beta=1}^3 (\xi + \mathbf{A}_\alpha \dot{q}_\alpha)^T \mathbb{I} (\xi + \mathbf{A}_\beta \dot{q}_\beta) + \frac{1}{2} d_{\alpha\beta} \dot{q}_\alpha \dot{q}_\beta. \quad (77)$$

Following (50) the body angular momentum is given by

$$\mathbf{J} = \mathbf{g}^T \mathbf{L} = \mathbf{r}_1 \times \mathbf{v}_1 + \mathbf{r}_2 \times \mathbf{v}_2. \quad (78)$$

Then by Eq. (71) and one has

$$\mathbf{J} = \mathbb{I} \cdot \left(\boldsymbol{\xi} + \sum_{\alpha=1}^3 \mathbf{A}_\alpha \dot{q}_\alpha \right). \quad (79)$$

The conjugate momenta are given by

$$\eta = \frac{\partial K}{\partial \boldsymbol{\xi}} = \mathbb{I} \cdot \left(\boldsymbol{\xi} + \sum_{\alpha=1}^3 \mathbf{A}_\alpha \dot{q}_\alpha \right) = \mathbf{J}, \quad (80)$$

and

$$p_\alpha = \frac{\partial K}{\partial \dot{q}_\alpha} = \sum_{\beta=1}^3 d_{\alpha\beta} \dot{q}_\beta + \mathbf{J}^T \mathbf{A}_\alpha. \quad (81)$$

Thus the Hamiltonian takes the form

$$h = \frac{1}{2} \mathbf{J}^T \mathbb{I}^{-1} \mathbf{J} + \frac{1}{2} \sum_{\alpha,\beta=1}^3 d^{\alpha\beta} (p_\alpha - \mathbf{J}^T \mathbf{A}_\alpha) (p_\beta - \mathbf{J}^T \mathbf{A}_\beta) + V, \quad (82)$$

where $V = V(q_1, q_2, q_3)$ is the potential.

Let us now make the expressions above more explicit by introducing coordinates. As the shape coordinates (q_1, q_2, q_3) we choose *Jacobi coordinates* (r_1, r_2, ϕ) which are defined as [3]

$$r_1 = \sqrt{\mathbf{r}_1 \cdot \mathbf{r}_1}, \quad r_2 = \sqrt{\mathbf{r}_2 \cdot \mathbf{r}_2}, \quad \phi = \cos^{-1}(\mathbf{r}_1 \cdot \mathbf{r}_2 / (r_1 r_2)), \quad (83)$$

$$0 \leq \phi \leq \pi,$$

(see Fig. 1). Choosing then the axes x_b, y_b, z_b of a body-fixed frame according to the so called *xyy-gauge*¹ shown in Fig. 2, one obtains for the moment of inertia tensor, metric and mechanical connection [3]

$$\mathbb{I} = \begin{bmatrix} r_2^2 \sin^2 \phi & -r_2^2 \sin \phi \cos \phi & 0 \\ -r_2^2 \sin \phi \cos \phi & r_1^2 + r_2^2 \cos^2 \phi & 0 \\ 0 & 0 & r_1^2 + r_2^2 \end{bmatrix}, \quad (84)$$

$$[d_{\mu\nu}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{r_1^2 r_2^2}{r_1^2 + r_2^2} \end{bmatrix}, \quad (85)$$

and

$$\mathbf{A}_{r_1} = \mathbf{A}_{r_2} = (0, 0, 0), \quad \mathbf{A}_\phi = \left(0, 0, \frac{r_2^2}{r_1^2 + r_2^2} \right), \quad (86)$$

respectively.

Putting the results above together the Hamiltonian in terms of Jacobi coordinates becomes

$$\begin{aligned} h(r_1, r_2, \phi, p_1, p_2, p_3, \mathbf{J}) \\ = \frac{1}{2} \left\{ \frac{r_1^2 + r_2^2 \cos^2 \phi}{r_1^2 r_2^2 \sin^2 \phi} J_1^2 + \frac{2 \cos \phi}{r_1^2 \sin \phi} J_1 J_2 + \frac{1}{r_1^2} J_2^2 + \frac{1}{r_1^2 + r_2^2} J_3^2 \right. \\ \left. + p_1^2 + p_2^2 + \frac{r_1^2 + r_2^2}{r_1^2 r_2^2} \left(p_3 - \frac{r_2^2}{r_1^2 + r_2^2} J_3 \right)^2 \right\} + V(r_1, r_2, \phi), \end{aligned}$$

where $\mathbf{J} = (J_1, J_2, J_3)$. Here $\|\mathbf{J}\|$ is conserved so the coadjoint orbit is the body angular momentum sphere $S^2(\|\mathbf{J}\|)$. One choice

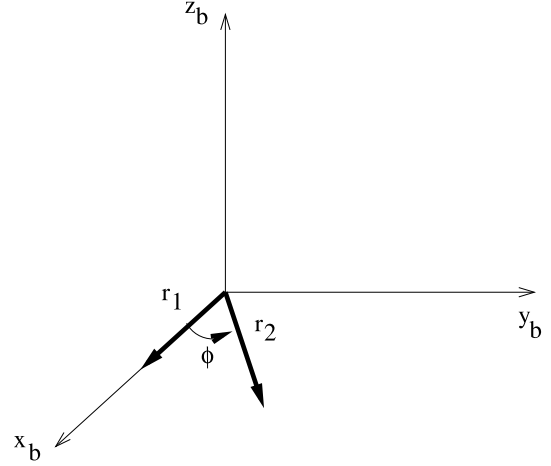


Fig. 2. Definition of a body-fixed frame according to the xyy-gauge.

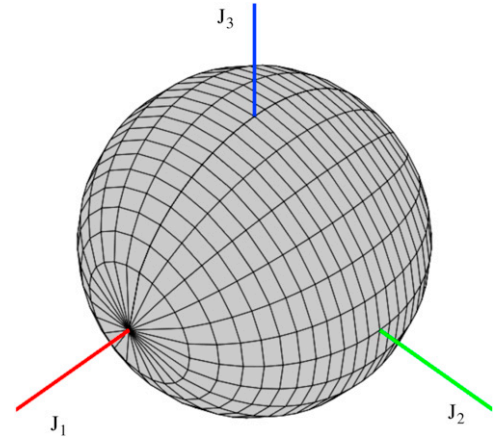


Fig. 3. Coordinate lines on the angular momentum sphere of (u, v) defined according to (87).

of canonical coordinates on $S^2(\|\mathbf{J}\|)$ are the so called *Deprit coordinates* which are defined as [34]

$$(J_1, J_2, J_3) = (v, \sqrt{r^2 - v^2} \sin u, \sqrt{r^2 - v^2} \cos u), \quad (87)$$

where $r = \|\mathbf{J}\|$ (see Fig. 3), then the reduced Hamiltonian $h|_{S^2(r)}$ becomes

$$\begin{aligned} h_r(r_1, r_2, \phi, p_1, p_2, p_3, u, v) \\ = \frac{1}{2} \left\{ \frac{r_1^2 + r_2^2 \cos^2 \phi}{r_1^2 r_2^2 \sin^2 \phi} v^2 + \frac{2 \cos \phi}{r_1^2 \sin \phi} v \sqrt{r^2 - v^2} \sin u \right. \\ \left. + \frac{1}{r_1^2} (r^2 - v^2) \sin^2 u + \frac{1}{r_1^2 + r_2^2} (r^2 - v^2) \cos^2 u + p_1^2 + p_2^2 \right. \\ \left. + \frac{r_1^2 + r_2^2}{r_1^2 r_2^2} \left(p_3 - \frac{r_2^2}{r_1^2 + r_2^2} \sqrt{r^2 - v^2} \cos u \right)^2 \right\} + V. \end{aligned}$$

4.2. Lagrangian equilateral triangle configurations

As a concrete example of a three-body system we choose the Morse-type potential given by

$$V = \sum_{1 \leq i < j \leq 3} \exp(-2(r_{ij} - d_0)) - 2 \exp(-(r_{ij} - d_0)), \quad (88)$$

¹ We note that the choice of a body-fixed frame corresponds to the choice of the local section σ of the fiber bundle $M \rightarrow Q$ in Section 3.4. The gauge theoretical interpretation of this choice is studied in great detail in [3].

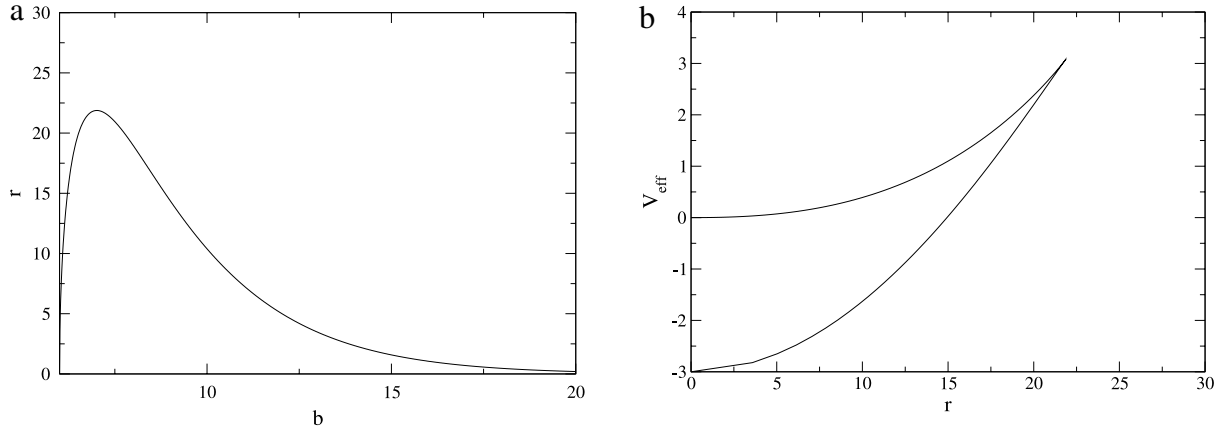


Fig. 4. (a) The magnitude r of the angular momentum as a function of the size of the Lagrangian equilateral triangle parametrized by b (see (92)). (b) The energy as given by the effective potential $V_{\text{eff}} = \frac{1}{2} \frac{r^2}{r_1^2 + r_2^2} + V$ (see (96)) for the Lagrangian relative equilibria as a function of r .

where r_{ij} is the distance between the i th and the j th particles. The parameter d_0 determines the side length of the equilateral triangle at which the potential has a minimum. In Jacobi coordinates one has

$$r_{13} = \frac{r_1}{\sqrt{\mu_1}}, \quad (89)$$

$$r_{23} = \sqrt{\frac{\mu_1 r_1^2}{m_3^2} + \frac{r_2^2}{\mu_2} + \frac{2\sqrt{\mu_1} r_1 r_2 \cos \phi}{m_3 \sqrt{\mu_2}}}, \quad (90)$$

$$r_{12} = \sqrt{\frac{\mu_1 r_1^2}{m_1^2} + \frac{r_2^2}{\mu_2} - \frac{2\sqrt{\mu_1} r_1 r_2 \cos \phi}{m_1 \sqrt{\mu_2}}}. \quad (91)$$

A Lagrangian equilateral triangle relative equilibrium is a planar motion where the shape is a constant equilateral triangle. The angular momentum is orthogonal to the plane of the motion. The mass-weighted Jacobi vectors are then of the form

$$\begin{aligned} \mathbf{r}_1^e &= \sqrt{\mu_1}(b, 0, 0), \\ \mathbf{r}_2^e &= \sqrt{\mu_2} \left(\frac{b}{2} \left(\frac{m_3 - m_1}{m_1 + m_3} \right), \pm \frac{\sqrt{3}}{2} b, 0 \right), \end{aligned} \quad (92)$$

where the parameter b is determined by the magnitude of the angular momentum r or conversely, choosing a value for b determines r . The corresponding Jacobi coordinates (r_1^e, r_2^e, ϕ^e) are easily computed using (83).

Now we find the values of the other coordinates and the parameter r at the equilibria specified by b . Following (82) a relative equilibrium satisfies [37]

$$\mathbf{J} \times (\mathbb{I}^{-1} \cdot \mathbf{J}) = 0, \quad (93)$$

$$p_\alpha = \mathbf{J} \cdot \mathbf{A}_\alpha, \quad (94)$$

$$\frac{\partial}{\partial q_\alpha} \left(\frac{1}{2} \mathbf{J}^T \mathbb{I}^{-1} \mathbf{J} + V \right) = 0. \quad (95)$$

By Eq. (93) \mathbf{J} is an eigenvector of \mathbb{I}^{-1} at a relative equilibrium point. For a Lagrangian equilateral triangle relative equilibrium, we know that in the xy -gauge (see Fig. 2) \mathbf{J} is pointing in the z -direction of the body frame. Hence $\mathbf{J} = (0, 0, r)$. From (87) we find the corresponding canonical coordinates $(u^e, v^e) = (0, 0)$. Inserting $\mathbf{J} = (0, 0, r)$ and using the block structure of the inertia tensor in (84) Eq. (95) reduces to

$$\frac{\partial}{\partial q_\alpha} \left(\frac{1}{2} \frac{r^2}{r_1^2 + r_2^2} + V \right) = 0. \quad (96)$$

We use this equation to find the magnitude of the angular momentum r for a Lagrangian equilateral triangle (r_1^e, r_2^e, ϕ^e) specified by a given parameter b in (92). Finally, inserting (86) in (94) the conjugate momenta are obtained to be

$$p_1^e = p_2^e = 0, \quad p_3^e = \frac{(r_2^e)^2}{(r_1^e)^2 + (r_2^e)^2} r. \quad (97)$$

Fig. 4a shows the magnitude of the angular momentum r as a function of the Lagrangian equilateral triangle specified by b . One sees that for a given value of r , there are two (or no) Lagrangian equilateral triangle of different sizes. The corresponding energies given by the effective potential $V_{\text{eff}} = \frac{1}{2} \frac{r^2}{r_1^2 + r_2^2} + V$ at these equilibria are shown in Fig. 4b. For a given value of r , the smaller Lagrangian triangle has the smaller energy.

As mentioned above at a relative equilibrium point the body angular momentum vector \mathbf{J} is an eigenvector of \mathbb{I}^{-1} . So, when looking for relative equilibria in general one would like to diagonalize \mathbb{I}^{-1} which is possible when passing to a principal axes frame. We note that the corresponding shape coordinates are called *Dracht's coordinates* [3,20]. As we were only interested in Lagrangian equilateral triangle configurations in this paper, the commonly used Jacobi coordinates were also useful in the study of these relative equilibria since \mathbb{I}^{-1} is diagonal in the third component which corresponds to the direction of the body fixed angular momentum in the xy -gauge.

4.3. Normal form around Lagrangian equilateral triangle relative equilibria

We now apply the procedure explained in Section 3.6 to compute the Poincaré–Birkhoff normal form around the Lagrangian equilibria. We choose unit masses, the parameter d_0 in the Morse potential in (88) equal to 6 and the parameter b specifying the side length of the Lagrangian equilateral triangle in (92) equal to 6.5. This gives the Jacobi coordinates

$$\begin{aligned} q_1^e &\equiv r_1^e = \sqrt{\mu_1} b = \frac{6.5}{\sqrt{2}}, \\ q_2^e &\equiv r_2^e = \sqrt{\mu_2} b \sqrt{\frac{3}{4}} = \frac{6.5}{\sqrt{2}}, \\ q_3^e &\equiv \phi^e = \frac{\pi}{2}. \end{aligned} \quad (98)$$

Solving (96) for r we find $r^e = 19.8302179854$.

The momenta conjugate to the Jacobi coordinates are

$$\begin{aligned} p_1^e &= 0, \\ p_2^e &= 0, \\ p_3^e &= \frac{(r_2^e)^2}{(r_1^e)^2 + (r_2^e)^2} r = 9.9151089927. \end{aligned} \quad (99)$$

The eigenvalues of the matrix $\mathfrak{J}D^2h_r$ that gives the linearized vector field are

$$\begin{aligned} \pm i\omega_1 &= \pm i 0.2362174000, \\ \pm i\omega_2 &= \pm i 0.4693542718, \\ \pm i\omega_3 &= \pm i 1.1749259437, \\ \pm i\omega_4 &= \pm i 1.1984363284. \end{aligned} \quad (100)$$

So we can immediately read off that the equilibrium is of elliptic linear stability. We note that a well established method for determining the stability of reduced systems is the *reduced energy-momentum method* which was introduced in [40]. For an application to the three-body problem, see also [43]. The reduced energy-momentum method does however not provide a means to compute higher order normal forms as we will do now.

Since we are only interested in demonstrating the basic principle of a normal form computation we will restrict ourselves to the normal of order 4. We start from the fourth order Taylor expansion of the Hamiltonian h_r at the relative equilibrium. It has 212 nonvanishing terms and we refrain from writing them down. The symplectic matrix M which yields the linear symplectic transformation after which the quadratic part of the Hamiltonian assumes the form

$$h_{r,2}^{(2)} = \sum_{k=1}^4 \omega_k (p_k^2 + q_k^2) \quad (101)$$

can be defined as

$$M = [c_1 \text{Re } \mathbf{v}_1, c_2 \text{Re } \mathbf{v}_2, c_3 \text{Re } \mathbf{v}_3, c_4 \text{Re } \mathbf{v}_4, c_1 \text{Im } \mathbf{v}_1, c_2 \text{Im } \mathbf{v}_2, c_3 \text{Im } \mathbf{v}_3, c_4 \text{Im } \mathbf{v}_4] \quad (102)$$

where the column vectors are the real and imaginary parts of the eigenvectors \mathbf{v}_k of $\mathfrak{J}D^2h_r$ for the eigenvalues $i\omega_k$ with coefficients

$$c_k = \frac{1}{\sqrt{\text{Re } \mathbf{v}_k \cdot \mathfrak{J} \text{Im } \mathbf{v}_k}}, \quad k = 1, \dots, 4. \quad (103)$$

We find that the matrix M is given by Box I.

Following the next step in the normal form procedure we find that the normal form of order 4 is given by

$$\begin{aligned} h_{r,\text{NF}}^{(4)} &= 2.1181531267 + 0.2362174000 I_1 + 0.4693542718 I_2 \\ &\quad + 1.1749259437 I_3 + 1.1984363284 I_4 \\ &\quad - 1.4978871558 I_1^2 - 7.7221894156 I_1 I_4 \\ &\quad - 0.9580186364 I_4^2 + 6.4183166825 I_1 I_3 \\ &\quad - 8.1361397396 I_3 I_4 - 0.8641444715 I_3^2 \\ &\quad - 0.2175152611 I_1 I_2 - 0.2069751620 I_2 I_4 \\ &\quad - 0.1815241432 I_2 I_3 + 0.0089977794 I_2^2. \end{aligned} \quad (105)$$

The Hamiltonian $h_{r,\text{NF}}^{(4)}$ is obtained from the general approach described in this paper. It yields an integrable nonlinear approximation of the 3-body problem reduced by the non-Abelian symmetry group $SO(3)$ which can be used to study the motion in the neighborhood of the Lagrangian equilateral relative equilibria. Higher order terms can be obtained following the normal form procedure. The computations of the eigenvalues and eigenvectors and the Taylor expansion were carried out using the computer algebra package Maple. The normalization computations were done using a C++

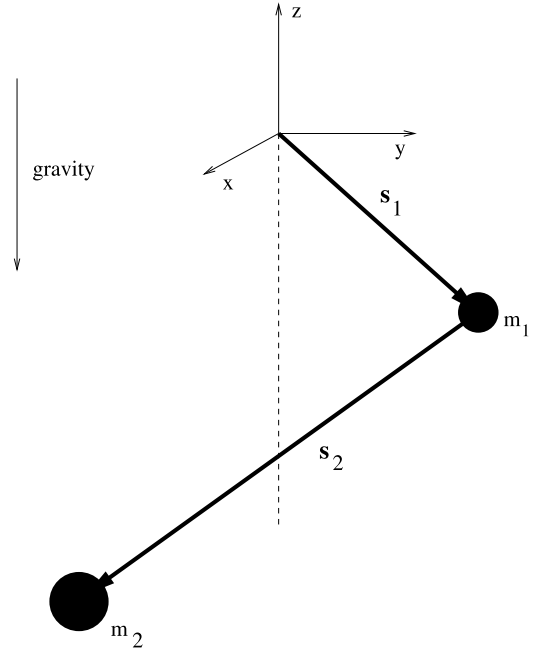


Fig. 5. The double spherical pendulum.

program written by one of the authors following the algorithm described in [41].

5. The double spherical pendulum

In this section we study the reduction of the double spherical pendulum (for a more detailed survey, we refer to [39]). We again introduce canonical coordinates on the reduced space in the light of Section 3. We use these to compute the Poincaré–Birkhoff normal form at the relative equilibrium given by a so called stretched-out solution.

5.1. Reduced equations of motion

Consider two coupled spherical pendula with masses m_1 and m_2 and position vectors \mathbf{s}_1 and \mathbf{s}_2 defined as in Fig. 5, moving without friction under the influence of a gravitational force $-a\mathbf{k}$ where a is a positive constant and \mathbf{k} is the unit vector in the z -direction.

If the lengths of \mathbf{s}_1 and \mathbf{s}_2 are l_1 and l_2 , respectively, then the configuration space is $M = S^2(l_1) \times S^2(l_2)$. The Lagrangian is

$$L(\mathbf{s}_1, \mathbf{s}_2, \dot{\mathbf{s}}_1, \dot{\mathbf{s}}_2) = \frac{1}{2} m_1 \|\dot{\mathbf{s}}_1\|^2 + \frac{1}{2} m_2 \|\dot{\mathbf{s}}_1 + \dot{\mathbf{s}}_2\|^2 \quad (106)$$

$$- m_1 a \mathbf{s}_1^T \mathbf{k} - m_2 a (\mathbf{s}_1 + \mathbf{s}_2)^T \mathbf{k}. \quad (107)$$

The system is invariant under rotations around the z -axis. So the symmetry group is the Abelian group $SO(2) \cong S^1$ whose action on M is given by

$$(\mathbf{s}_1, \mathbf{s}_2) \rightarrow (g_\theta \mathbf{s}_1, g_\theta \mathbf{s}_2), \quad (108)$$

where g_θ is the rotation by the angle θ about the z -axis. We can identify the Lie algebra of S^1 with $\text{span}(\mathbf{k})$. An element of the Lie algebra is then an angular velocity vector of the form $\omega\mathbf{k}$ with $\omega \in \mathbb{R}$ and the corresponding fundamental vector field is $\omega(\mathbf{k} \times \mathbf{s}_1, \mathbf{k} \times \mathbf{s}_2)$. For the angular momentum, we find according to (8)

$$\begin{aligned} \langle L(\mathbf{s}_1, \mathbf{s}_2, \dot{\mathbf{s}}_1, \dot{\mathbf{s}}_2), \omega\mathbf{k} \rangle &= \omega(m_1 \dot{\mathbf{s}}_1^T (\mathbf{k} \times \mathbf{s}_1) \\ &\quad + m_2 (\dot{\mathbf{s}}_1 + \dot{\mathbf{s}}_2)^T (\mathbf{k} \times \mathbf{s}_1 + \mathbf{k} \times \mathbf{s}_2)) \end{aligned} \quad (109)$$

or

$$\mathbf{L} = [\mathbf{k}^T (m_1 (\mathbf{s}_1 \times \dot{\mathbf{s}}_1) + m_2 (\mathbf{s}_1 + \mathbf{s}_2) \times (\dot{\mathbf{s}}_1 + \dot{\mathbf{s}}_2))] \mathbf{k}. \quad (110)$$

$$\begin{pmatrix} 0 & 0.2245619939 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.5952500442 & 0 & 0.5952500442 & -0.6459181965 & 0 & 0 & 0 & 0 \\ -0.5952500442 & 0 & -0.5952500442 & -0.6459181965 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.2590186725 & 0 & -0.2590186725 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4.4531132913 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.1406084178 & 0 & 0.6993747200 & -0.7740918318 \\ 0 & 0 & 0 & 0 & -0.1406084178 & 0 & -0.6993747200 & -0.7740918318 \\ -3.2144619462 & 0 & 0.6462635772 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \quad (104)$$

Box I.

If the body frame is chosen such that the x -axis coincides with \mathbf{s}_1^\perp , where \mathbf{s}_1^\perp is the projection of \mathbf{s}_1 onto xy -plane, and if we introduce polar coordinates (r, θ) in the xy -plane then we obtain for the body-fixed position vectors

$$\mathbf{r}_1 = (r_1, 0, -\sqrt{l_1^2 - r_1^2}), \quad (111)$$

$$\mathbf{r}_2 = (r_2 \cos \varphi, r_2 \sin \varphi, -\sqrt{l_2^2 - r_2^2}). \quad (112)$$

Note that through the choice of the sign of the square roots in the last components these equations are restricted to downward pointing configurations. As r_1, r_2, φ are invariant under the group action we can take them as shape coordinates on the three-dimensional shape space $Q = S^2(l_1) \times S^2(l_2)/S^1$.

The moment of inertia tensor

$$\mathbb{I} = m_1 \|\mathbf{r}_1^\perp\|^2 + m_2 \|(\mathbf{r}_1 + \mathbf{r}_2)^\perp\|^2, \quad (113)$$

where \mathbf{r}_1^\perp is the projection of \mathbf{r}_1 onto the xy -plane, can be written in terms of the shape coordinates as

$$\mathbb{I} = (m_1 + m_2)r_1^2 + 2m_2r_1r_2 \cos \varphi + m_2r_2^2. \quad (114)$$

Accordingly, we get for the mechanical connection

$$\begin{aligned} A_{r_1} &= -\frac{m_1m_2r_2 \sin \varphi}{\mathbb{I}}, & A_{r_2} &= \frac{m_1m_2r_1 \sin \varphi}{\mathbb{I}}, \\ A_\varphi &= \frac{m_1m_2r_2(r_1 \cos \varphi + r_2)}{\mathbb{I}}, \end{aligned} \quad (115)$$

and the entries of the matrix d which gives the horizontal metric are

$$\begin{aligned} d_{11} &= \frac{l_1^2(m_1 + m_2)}{2(l_1^2 - r_1^2)} - \frac{m_1^2m_2^2r_2^2 \sin^2 \varphi}{(m_1 + m_2)r_1^2 + 2m_2r_1r_2 \cos \varphi + m_2r_2^2}, \\ d_{12} &= \frac{1}{2}m_2 \left(\cos \varphi + r_1r_2 \left(\frac{1}{\sqrt{l_1^2 - r_1^2}\sqrt{l_2^2 - r_2^2}} \right. \right. \\ &\quad \left. \left. + \frac{2m_1^2m_2 \sin^2 \varphi}{(m_1 + m_2)r_1^2 + 2m_2r_1r_2 \cos \varphi + m_2r_2^2} \right) \right), \\ d_{13} &= \frac{1}{2}m_2r_2 \left(-1 \right. \\ &\quad \left. + \frac{2m_1^2m_2r_2(r_1 \cos \varphi + r_2)}{(m_1 + m_2)r_1^2 + 2m_2r_1r_2 \cos \varphi + m_2r_2^2} \right) \sin \varphi, \\ d_{22} &= m_2 \left(\frac{l_2^2}{2(l_2^2 - r_2^2)} - \frac{m_1^2m_2r_1^2 \sin^2 \varphi}{(m_1 + m_2)r_1^2 + 2m_2r_1r_2 \cos \varphi + m_2r_2^2} \right), \\ d_{23} &= -\frac{m_1^2m_2^2r_1r_2(r_1 \cos \varphi + r_2 \sin \varphi)}{(m_1 + m_2)r_1^2 + 2m_2r_1r_2 \cos \varphi + m_2r_2^2}, \\ d_{33} &= m_2r_2^2 \left(1 - \frac{m_1^2m_2(r_1 \cos \varphi + r_2)^2}{(m_1 + m_2)r_1^2 + 2m_2r_1r_2 \cos \varphi + m_2r_2^2} \right). \end{aligned}$$

The left-action of the group on the tangent bundle is trivial, so $\mathbf{J} = \mathbf{L}$. The conjugate momenta of the shape coordinates are given by

$$p_\alpha = \frac{\partial L}{\partial q_\alpha} = \sum_{\beta=1}^3 g_{\alpha\beta} \dot{q}_\beta + \mathbf{J} \mathbf{A}_\alpha. \quad (116)$$

Thus the Hamiltonian takes the form

$$h = \frac{1}{2} \mathbb{I}^{-1} \mathbf{J}^2 + \frac{1}{2} \sum_{\alpha, \beta=1}^3 d^{\alpha\beta} (p_\alpha - \mathbf{J} \mathbf{A}_\alpha)(p_\beta - \mathbf{J} \mathbf{A}_\beta) + V, \quad (117)$$

where $V = -m_1 a \sqrt{l_1^2 - r_1^2} - m_2 a (\sqrt{l_1^2 - r_1^2} + \sqrt{l_2^2 - r_2^2})$ is the potential. Observe here that as \mathbf{L} is conserved, \mathbf{J} is also conserved and can be viewed as a parameter.

The reduced equations of motion are

$$\begin{aligned} \dot{q}_\alpha &= \frac{\partial h_r}{\partial p_\alpha} = d^{\alpha\beta} (p_\beta - \mathbf{J} \mathbf{A}_\beta), \\ \dot{p}_\alpha &= -\frac{\partial h_r}{\partial q_\alpha} \\ &= -\frac{\partial}{\partial q_\alpha} \left(\frac{1}{2} \mathbb{I}^{-1} \mathbf{J}^2 + d^{\alpha\beta} (p_\alpha - \mathbf{J} \mathbf{A}_\alpha)(p_\beta - \mathbf{J} \mathbf{A}_\beta) \right) + V(q), \end{aligned} \quad (118)$$

where we denote by r the z -component of the conserved angular momentum \mathbf{J} .

5.2. Relative equilibria

Because of the triviality of the coadjoint action the conditions to have a relative equilibrium (58) reduce to

$$\begin{aligned} p_\alpha &= \mathbf{J} \mathbf{A}_\alpha, \\ \frac{\partial}{\partial q_\alpha} \left(\frac{1}{2} \mathbb{I}^{-1} \mathbf{J}^2 + V(q) \right) &= 0. \end{aligned} \quad (119)$$

As shown in [39] there are two types of relative equilibria: the so called cowboy branch and the stretched-out solution that we will concentrate on in the following and which is shown in Fig. 6. For a stretched-out relative equilibrium, we have $\varphi = 0$. We find r_1 and r_2 from solving (119) (using the computer algebra program Maple). The corresponding momenta are obtained from (116). We will in the following choose all parameters to have unit values, i.e. $m_1 = l_1 = m_2 = l_2 = a = 1$. The energy of the stretched-out relative equilibrium as a function of \mathbf{J} for this choice of parameters is shown in Fig. 7a.

5.3. Normal form around stretched-out relative equilibria

The stretched-out relative equilibria are known to be stable [39]. In agreement with this result we find that the eigenvalues of the matrix $\mathfrak{J} D^2 h_r$ associated with the linearized vector field of the reduced system at the stretched-out relative equilibria are purely imaginary. The frequencies ω_k , $k = 1, 2, 3$, are shown in Fig. 7b as a function of r .

For the normal form computation, we consider the relative equilibrium point which has $r = 1$. For the position of this relative

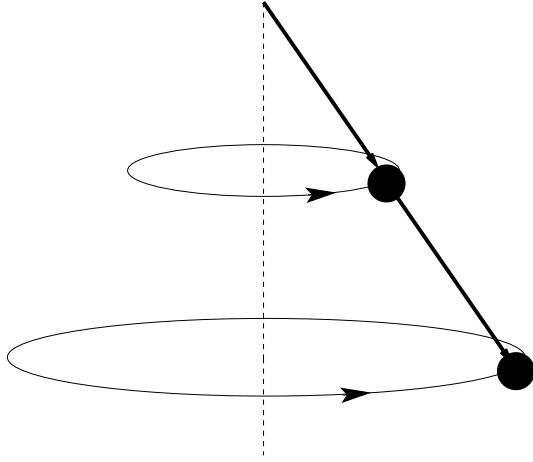


Fig. 6. A stretched-out relative equilibrium solution of the double spherical pendulum in which the two masses are aligned with the point of suspension and move along circles.

equilibrium, we find

$$\begin{aligned} q_1^e &\equiv r_1^e = 0.4425598655, \\ q_2^e &\equiv r_2^e = 0.5656579210 \\ q_3^e &\equiv \varphi^e = 0, \\ p_1 &= 0, \\ p_2 &= 0, \\ p_3 &= 0.4704091824. \end{aligned} \quad (120)$$

The Taylor expansion of the reduced Hamiltonian to order 4 has 186 nonvanishing terms at this relative equilibrium. The eigenvalues associated with the linearized vector field are

$$\begin{aligned} \pm i \omega_1 &= \pm i 1.2572610531, \\ \pm i \omega_2 &= \pm i 1.4864684140, \\ \pm i \omega_3 &= \pm i 2.6603546311. \end{aligned} \quad (121)$$

We define the symplectic matrix M which transforms the quadratic part of the Hamiltonian to the form $\sum_{k=1}^3 \omega_k(p_k^2 + q_k^2)$ analogously to (102) in Section 4.3. We find Eq. (122), given in Box II. Following the normal form procedure we get for the 4th order normal form

$$\begin{aligned} h_{r, \text{NF}}^{(4)} &= -2.2056999577 + 1.2572610531 I_1 \\ &+ 1.4864684140 I_2 + 2.6603546311 I_3 \\ &+ 0.0467015469 I_1^2 - 5.8213832524 I_1 I_3 \end{aligned}$$

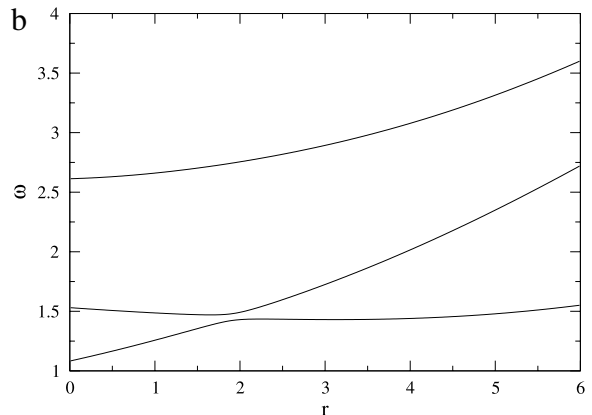
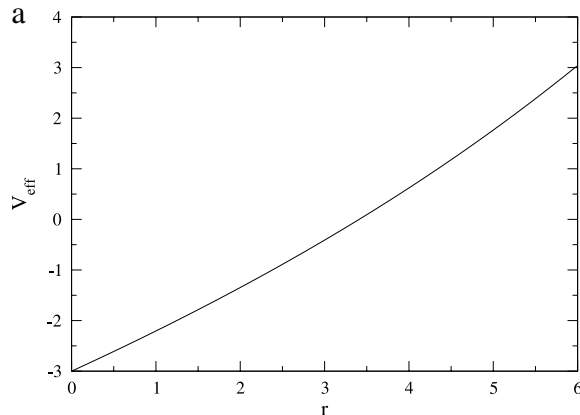


Fig. 7. (a) Energy of the stretched-out relative equilibrium as given by the effective or amended potential $V_{\text{eff}} = \frac{1}{2} \mathbb{I}^{-1} \mathbf{J}^2 + V(q)$ (see (119)) as a function of the angular momentum r . (b) Frequencies of the stretched-out relative equilibrium as a function of r .

$$\begin{aligned} &+ 0.0875786340 I_3^2 + 0.1772800788 I_1 I_2 \\ &- 0.0932948515 I_2 I_3 - 0.0419637147 I_2^2. \end{aligned} \quad (123)$$

The Hamiltonian $h_{r, \text{NF}}^{(4)}$ yields an integrable nonlinear approximation of the double spherical pendulum reduced by the Abelian symmetry group $SO(2)$ in the neighborhood of the stretched-out relative equilibrium. Similarly to the 3-body case in Section 4.3 the normal form of the reduced system is obtained from the general approach in this paper which demonstrates the effectiveness and generality of the approach. As described in Section 4.3 the computations were carried using Maple and a C++ program written by one of the authors.

6. Conclusions and outlook

In this paper we provided a general perspective on the construction of canonical coordinates for the reduced spaces of Hamiltonian systems given by cotangent bundles with a free Lie group action. The general approach presented in this paper allows one to treat the reduction of Abelian and non-Abelian group actions on the same footing. The case of simple mechanical systems was studied in detail. The approach was illustrated for a 3-body problem and the double spherical pendulum which involve non-Abelian and Abelian symmetries, respectively. We used the canonical coordinates to compute the Poincaré–Birkhoff normal forms at the relative equilibria given by the Lagrangian equilateral triangle configuration in the 3-body problem and the stretched-out solution of the double spherical pendulum. The Poincaré–Birkhoff normal form gives a nonlinear approximation of the local dynamics of the reduced system in the neighborhood of the relative equilibria. This goes beyond the well established reduced energy–momentum method which gives the stability of the relative equilibria [40] and enables one, e.g., to give nonlinear approximations of the center manifolds of relative equilibria. The use of a Poincaré–Birkhoff normal form for the computation of the center manifolds of saddle type equilibria has in recent years been demonstrated in the study of reaction type dynamics [10,11]. The study of this paper allows one to carry over these results to the case of saddle type relative equilibria which induce reaction type dynamics in rotating molecules [12]. In this context also the reconstruction of the full dynamics from the reduced one is of great interest. We leave this issue for a future paper and instead refer to [44,45] for some general background on this important problem.

In this paper we excluded Lie group actions with isotropy which have been studied, e.g., in [15] or [37,18] for the case of n -body systems. Our future studies concern how isotropy can be

$$M = \begin{pmatrix} 0.3720476175 & -0.3116300067 & 0.4202281883 & 0 & 0 & 0 \\ -0.5712604029 & -0.3238407419 & -0.5369033436 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2.2390869882 & -0.2974563002 & -2.2029538091 \\ 0 & 0 & 0 & -0.8426837965 & -1.6576611267 & 1.8964495311 \\ 0 & 0 & 0 & 0.3873035344 & -1.4365053634 & -1.4081719163 \\ -0.6854444155 & 0.0612664420 & -0.2510237658 & 0 & 0 & 0 \end{pmatrix}. \quad (122)$$

Box II.

incorporated in the approach presented in this paper to do, e.g., a normal form analysis for 3-body systems with linear equilibrium configurations. Another related problem is the development of a normal form algorithm which is coordinate independent or in the jargon of [3] *gauge independent*. This problem is considered in [46] and its generalizations to cotangent bundles in general seems worth studying.

Recently considerable progress was made in nonholonomic mechanics (see, e.g., [32,47] and the references therein). It might be possible to use these techniques to develop a non-canonical Poincaré–Birkhoff normal form related to the results of this paper.

Finally we mention that it would be interesting to transfer the results of this paper to quantum mechanical systems. Analogously to the Poincaré–Birkhoff normal form of an equilibrium point there is a quantum normal form built on the symbol calculus of pseudo differential operators by which one can locally approximate a quantum Hamilton operator. In the case of elliptic equilibria this allows one to compute quantum energy spectra with high precision. For saddle type equilibria, the quantum normal form can be used to compute efficiently quantum reaction rates and the associated Gamow–Siebert resonances (see [48,49] and also the references therein for quantum normal forms in general). It would be interesting to transfer these results to relative equilibria of rotational symmetry reduced molecular systems. The dependence of the quantization of quantum reaction rates in the hydrogen exchange reaction as a function of the angular momentum has, e.g., been studied in [50] using *ab initio* quantum computations. It would be interesting to compare these results to a quantum normal computation. The geometric approach for quantum 3-body problems presented in [20] could be very useful for this purpose.

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References

- [1] R. Abraham, J.E. Marsden, Foundations of Mechanics, Benjamin/Cummings Publishing Co. Inc., Reading, Mass, 1978.
- [2] J.E. Marsden, Lectures on Mechanics, Cambridge University Press, Cambridge, 1992.
- [3] R.G. Littlejohn, M. Reinsch, Gauge fields in the separation of rotations and internal motions in the n -body problem, Rev. Modern Phys. 69 (1997) 213–275.
- [4] A. Deprit, Canonical transformations depending on a small parameter, Celestial Mech. 1 (1969) 12–30.
- [5] V.I. Arnol'd, V.V. Kozlov, A.I. Neishtadt, Mathematical aspects of classical and celestial mechanics, in: V.I. Arnol'd (Ed.), Dynamical Systems III, in: Encyclopaedia of Mathematical Sciences, vol. 3, Springer, Berlin, 1988.
- [6] A.J. Dragt, J.M. Finn, Lie series and invariant functions for analytic symplectic maps, J. Math. Phys. 17 (12) (1976) 2215–2227.
- [7] J. Murdock, Normal forms and unfoldings for local dynamical systems, in: Springer Monographs in Mathematics, Springer-Verlag, New York, 2003.
- [8] H.W. Broer, Normal forms in perturbation theory, in: R.A. Meyers (Ed.), Encyclopedia of Complexity and Systems Science, Springer, 2009, pp. 6310–6329.
- [9] H. Hanßmann, Local and Semi-Local Bifurcations in Hamiltonian Dynamical Systems, Springer, Berlin, Heidelberg, 1978.
- [10] T. Uzer, C. Jaffé, J. Palacián, P. Yanguas, S. Wiggins, The geometry of reaction dynamics, Nonlinearity 15 (2002) 957–992.
- [11] H. Waalkens, A. Burbanks, S. Wiggins, Phase space conduits for reaction in multidimensional systems: HCN isomerization in three dimensions, J. Chem. Phys. 121 (13) (2004) 6207–6225.
- [12] Ü. Çiftçi, H. Waalkens, Phase space structures governing reaction dynamics in rotating molecules, Nonlinearity 25 (2012) 791–892.
- [13] K.A. Mitchell, R.G. Littlejohn, The rovibrational kinetic energy for complexes of rigid molecules, Mol. Phys. 96 (9) (1999) 1305–1315.
- [14] M. Roberts, C. Wulff, J.S.W. Lamb, Hamiltonian systems near relative equilibria, J. Differential Equations 179 (2) (2002) 562–604.
- [15] M. Roberts, T. Schmäh, C. Stoica, Relative equilibria in systems with configuration space isotropy, J. Geom. Phys. 56 (5) (2006) 762–779.
- [16] J.E. Marsden, J. Scheurle, The reduced Euler–Lagrange equations, in: Dynamics and control of mechanical systems (Waterloo, ON, 1992), in: Fields Inst. Commun., vol. 1, Amer. Math. Soc, Providence, RI, 1993, pp. 139–164.
- [17] Wang Sang Koon, Jerrold E. Marsden, The Hamiltonian and Lagrangian approaches to the dynamics of nonholonomic systems, Rep. Math. Phys. 40 (1) (1997) 21–62.
- [18] T. Iwai, H. Yamaoka, Stratified reduction of classical many-body systems with symmetry, J. Phys. A: Math. Gen. 38 (2005) 2415–2439.
- [19] J.E. Marsden, G. Misiołek, J.-P. Ortega, M. Perlmutter, T.S. Ratiu, Hamiltonian Reduction by Stages, Vol. 1913, Springer, Berlin, 2007.
- [20] T. Iwai, A geometric setting for internal motions of the quantum three-body system, J. Math. Phys. 28 (6) (1987) 1315–1326.
- [21] K.R. Meyer, G.R. Hall, Introduction to Hamiltonian Dynamical Systems and the N -Body Problem, Springer, Berlin, 1992.
- [22] R.C. Churchill, M. Kummer, D.L. Rod, On averaging, reduction, and symmetry in Hamiltonian systems, J. Differential Equations 49 (3) (1983) 359–414.
- [23] À. Jorba, J. Villanueva, Numerical computation of normal forms around some periodic orbits of the restricted three-body problem, Physica D 114 (3–4) (1998) 197–229.
- [24] G. Gómez, W.S. Koon, M.W. Lo, J.E. Marsden, J. Masdemont, S.D. Ross, Connecting orbits and invariant manifolds in the spatial restricted three-body problem, Nonlinearity 17 (5) (2004) 1571–1606.
- [25] A. Chenciner, J. Féjoz, The flow of the equal-mass spatial 3-body problem in the neighborhood of the equilateral relative equilibrium, Discrete Contin. Dyn. Syst. Ser. B 10 (2–3) (2008) 421–438.
- [26] L. Chierchia, G. Pinzari, The planetary N -body problem: symplectic foliation, reductions and invariant tori, Invent. Math. 186 (1) (2011) 1–77.
- [27] J.S.W. Lamb, I. Melbourne, Normal form theory for relative equilibria and relative periodic solutions, Trans. Amer. Math. Soc. 359 (9) (2007) 4537–4556.
- [28] V.I. Arnol'd, Mathematical Methods of Classical Mechanics, in: Graduate Texts in Mathematics, vol. 60, Springer, Berlin, 1978.
- [29] J.-P. Ortega, T.S. Ratiu, Momentum Maps and Hamiltonian Reduction, Birkhäuser Boston Inc., Boston, MA, 2004.
- [30] G.-M. Marle, Symplectic manifolds, dynamical groups, and Hamiltonian mechanics, in: Differential Geometry and Relativity, in: Mathematical Phys. and Appl. Math., vol. 3, Reidel, Dordrecht, 1976, pp. 249–269.
- [31] J.A. Montaldi, R.M. Roberts, Relative equilibria of molecules, J. Nonlinear Sci. 9 (1) (1999) 53–88.
- [32] A.M. Bloch, P.S. Krishnaprasad, J.E. Marsden, R.M. Murray, Nonholonomic mechanical systems with symmetry, Arch. Ration. Mech. Anal. 136 (1) (1996) 21–99.
- [33] W.W. Symes, Hamiltonian group actions and integrable systems, Physica D 1 (4) (1980) 339–374.
- [34] A. Deprit, Free Rotation of a Rigid Body Studied in the Phase Plane, Amer. J. Phys. 35 (1967) 424–428.
- [35] R. Montgomery, Gauge theory of the falling cat, in: Dynamics and Control of Mechanical Systems (Waterloo, ON, 1992), in: Fields Inst. Commun., vol. 1, Amer. Math. Soc, Providence, RI, 1993, pp. 193–218.
- [36] I.N. Kozin, R.M. Roberts, J. Tennyson, Symmetry and structure of rotating H_2^+ , J. Chem. Phys. 111 (1999) 140–150.
- [37] I.N. Kozin, R.M. Roberts, J. Tennyson, Relative equilibria of D_2H^+ and H_2D^+ , Mol. Phys. 98 (2000) 295–307.
- [38] H. Cendra, J.E. Marsden, S. Pekarsky, T.S. Ratiu, Variational principles for Lie–Poisson and Hamilton–Poincaré equations, Mosc. Math. J. 3 (3) (2003) 833–867.

- [39] J.E. Marsden, J. Scheurle, Lagrangian reduction and the double spherical pendulum, *Z. Angew. Math. Phys.* 44 (1) (1993) 17–43.
- [40] J.C. Simo, D. Lewis, J.E. Marsden, Stability of relative equilibria. I. The reduced energy-momentum method, *Arch. Ration. Mech. Anal.* 115 (1) (1991) 15–59.
- [41] P. Collins, A. Burbanks, S. Wiggins, H. Waalkens, R. Schubert, Bristol University normal form software, 2008.
<http://lacms.maths.bris.ac.uk/publications/software>.
- [42] Ü. Çiftçi, H. Waalkens, Holonomy-reduced dynamics of triatomic molecules, *J. Phys. A* 44 (2011) 165202.
- [43] T. Schmäh, C. Stoica, Stability for Lagrangian relative equilibria of three-point-mass systems, *J. Phys. A* 39 (46) (2006) 14405–14425.
- [44] J. Marsden, R. Montgomery, T. Ratiu, Reduction, symmetry, and phases in mechanics, *Mem. Amer. Math. Soc.* 88 (436) (1990).
- [45] R. Montgomery, The geometric phase of the three-body problem, *Nonlinearity* 9 (5) (1996) 1341–1360.
- [46] R.G. Littlejohn, K.A. Mitchell, Gauge theory of small vibrations in polyatomic molecules, in: *Geometry, Mechanics, and Dynamics*, Springer, New York, 2002, pp. 407–428.
- [47] A.M. Bloch, J.E. Marsden, D.V. Zenkov, Quasivelocities and symmetries in non-holonomic systems, *Dyn. Syst.* 24 (2) (2009) 187–222.
- [48] R. Schubert, H. Waalkens, S. Wiggins, Efficient computation of transition state resonances and reaction rates from a quantum normal form, *Phys. Rev. Lett.* 96 (2006) 218302.
- [49] H. Waalkens, R. Schubert, S. Wiggins, Wigner's dynamical transition state theory in phase space: classical and quantum, *Nonlinearity* 21 (1) (2008) R1–R118.
- [50] D.C. Chatfield, S.L. Mielke, T.C. Allison, D.G. Truhlar, Quantized dynamical bottlenecks and transition state control of the reaction of D with H₂: effect of varying the total angular momentum, *J. Chem. Phys.* 112 (19) (2000) 8387–8408.